Karl F Freed

List of Publications by Year
in descending order

616 papers	21,348 citations	10389 72 h-index	30922 102 g-index
626 all docs	626 docs citations	626 times ranked	7760 citing authors

#	Article	IF	Citations
1	Prediction and Validation of a Proteinâ€™s Free Energy Surface Using Hydrogen Exchange and (Importantly) Its Denaturant Dependence. Journal of Chemical Theory and Computation, 2022, 18, 550-561.	5.3	8
2	Challenges and Advantages of Accounting for Backbone Flexibility in Prediction of Proteinâ€"Protein Complexes. Journal of Chemical Theory and Computation, 2022, 18, 2016-2032.	5.3	2
3	Lattice theory for binding of linear polymers to a solid substrate from polymer melts. II. Influence of van der Waals interactions and chain semiflexibility on molecular binding and adsorption. Journal of Chemical Physics, 2019, 151, 124709.	3.0	3
4	Lattice theory for binding of linear polymers to a solid substrate from polymer melts: I. Influence of chain connectivity on molecular binding and adsorption. Journal of Chemical Physics, 2019, 151, 124706.	3.0	3
5	On the Interpretation of Force-Induced Unfolding Studies of Membrane Proteins Using Fast Simulations. Biophysical Journal, 2019, 117, 1429-1441.	0.5	12
6	The Effect of Amyloid Precursor Protein Dimerization on its Conformation and Cleavage. Biophysical Journal, 2019, 116, 495a.	0.5	0
7	Fast, Atomic-Level AFM and Magnetic Tweezers Simulations of the Unfolding of Membrane Proteins using a New Membrane Burial Potential with H-Bonding. Biophysical Journal, 2019, 116, 300a-301a.	0.5	0
8	A Multi-scale Study of Î²-Amyloid Wild-Type and Mutant Peptides: Monomers, Oligomers, Fibrils. Biophysical Journal, 2018, 114, 430a-431a.	0.5	0
9	Amyloid-Î² Peptide Interaction with Lipid Bilayer Promotes Peptide Aggregation on the Surface and Modulates Lipid Behavior. Biophysical Journal, 2018, 114, 429a-430a.	0.5	0
10	Upside: A New Dynamics Methods Capable of Cooperative De Novo Protein Folding in CPU-Hours. Biophysical Journal, 2018, 114, 677a.	0.5	0
11	A Membrane Burial Potential with H-Bonds and Applications to Curved Membranes and Fast Simulations. Biophysical Journal, 2018, 115, 1872-1884.	0.5	9
12	Accurate calculation of side chain packing and free energy with applications to protein molecular dynamics. PLoS Computational Biology, 2018, 14, e1006342.	3.2	31
13	Trajectory-based training enables protein simulations with accurate folding and Boltzmann ensembles in cpu-hours. PLoS Computational Biology, 2018, 14, e1006578.	3.2	33
14	Response to Comment on â€œInnovative scattering analysis shows that hydrophobic disordered proteins are expanded in waterâ€• Science, 2018, 361, .	12.6	30
15	Lattice theory of competitive binding: Influence of van der Waals interactions on molecular binding and adsorption to a solid substrate from binary liquid mixtures. Journal of Chemical Physics, 2018, 149, 044704.	3.0	6
16	Dielectric virial expansion of polarizable dipolar spheres. Journal of Chemical Physics, 2018, 149, 163332.	3.0	3
17	Measuring the solvent quality of water for disordered proteins from a single SAXS measurement. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a221-a221.	0.1	0
18	Influence of Pressure on Glass Formation in a Simulated Polymer Melt. Macromolecules, 2017, 50, 2585-2598.	4.8	34

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19	Comparative Study of the Collective Dynamics of Proteins and Inorganic Nanoparticles. Scientific Reports, 2017, 7, 41671.	3.3	12
20	Folding Membrane Proteins by Contacts Inferred from Non-Membrane Proteins and Near-Atomic Level Refinement. Biophysical Journal, 2017, 112, 204a-205a.	0.5	0
21	Measuring the (Good) Solvent Quality of Water for Disordered Proteins from a Single SAXS Measurement. Biophysical Journal, 2017, 112, 316a.	0.5	0
22	Membrane Bilayers Help to Stabilize and are Affected by AÎ²-Fibrils on the Surface: A Molecular Dynamics Study. Biophysical Journal, 2017, 112, 363a.	0.5	0
23	Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water. Science, 2017, 358, 238-241.	12.6	194
24	Mixtures of two self- and mutually-associating liquids: Phase behavior, second virial coefficients, and entropy-enthalpy compensation in the free energy of mixing. Journal of Chemical Physics, 2017, 147, 064909.	3.0	14
25	Image method for electrostatic energy of polarizable dipolar spheres. Journal of Chemical Physics, 2017, 147, 064908.	3.0	8
26	Self-assembly and glass-formation in a lattice model of telechelic polymer melts: Influence of stiffness of the sticky bonds. Journal of Chemical Physics, 2016, 144, 214903.	3.0	2
27	Stringlike Cooperative Motion Explains the Influence of Pressure on Relaxation in a Model Glass-Forming Polymer Melt. ACS Macro Letters, 2016, 5, 1375-1380.	4.8	22
28	Generalized entropy theory of glass-formation in fully flexible polymer melts. Journal of Chemical Physics, 2016, 145, 234509.	3.0	30
29	Including H-Bonding in Depth-Dependent Membrane Burial Potentials for Improving Folding Simulations. Biophysical Journal, 2016, 110, 58a.	0.5	1
30	Upside: A New Dynamics Method Capable of Cooperative De Novo Protein Folding in CPU-Hours. Biophysical Journal, 2016, 110, 523a-524a.	0.5	0
31	AÎ² Fibrils Act as Aqueous Pores: A Molecular Dynamics Study. Biophysical Journal, 2016, 110, 553a.	0.5	0
32	Cooperative folding near the downhill limit determined with amino acid resolution by hydrogen exchange. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4747-4752.	7.1	6
33	Influence of Cohesive Energy on the Thermodynamic Properties of a Model Glass-Forming Polymer Melt. Macromolecules, 2016, 49, 8341-8354.	4.8	65
34	Influence of Cohesive Energy on Relaxation in a Model Glass-Forming Polymer Melt. Macromolecules, 2016, 49, 8355-8370.	4.8	60
35	Image method for induced surface charge from many-body system of dielectric spheres. Journal of Chemical Physics, 2016, 145, 124903.	3.0	25
36	Relation Between Solvent Quality and Phase Behavior of Ternary Mixtures of Polymers and Two Solvents that Exhibit Cononsolvency. Journal of Physical Chemistry B, 2016, 120, 5753-5758.	2.6	9

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37	A theory of interactions between polarizable dielectric spheres. Journal of Colloid and Interface Science, 2016, 469, 237-241.	9.4	33
38	Surface Interactions Restricts Amyloid-Î² Peptides Movements Resulting in their Rapid Self-Assembly into Î² Sheets; a Molecular Dynamics Study. Biophysical Journal, 2015, 108, 64a.	0.5	0
39	Communication: The simplified generalized entropy theory of glass-formation in polymer melts. Journal of Chemical Physics, 2015, 143, 051102.	3.0	3
40	Communication: Cosolvency and cononsolvency explained in terms of a Flory-Huggins type theory. Journal of Chemical Physics, 2015, 143, 131101.	3.0	79
41	Lattice model of linear telechelic polymer melts. I. Inclusion of chain semiflexibility in the lattice cluster theory. Journal of Chemical Physics, 2015, 143, 024901.	3.0	4
42	Lattice model of linear telechelic polymer melts. II. Influence of chain stiffness on basic thermodynamic properties. Journal of Chemical Physics, 2015, 143, 024902.	3.0	3
43	Phase behavior and second osmotic virial coefficient for competitive polymer solvation in mixed solvent solutions. Journal of Chemical Physics, 2015, 143, 194901.	3.0	9
44	The meaning of the â€œuniversalâ€•WLF parameters of glass-forming polymer liquids. Journal of Chemical Physics, 2015, 142, 014905.	3.0	40
45	Even with nonnative interactions, the updated folding transition states of the homologs Proteins G & L are extensive and similar. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 8302-8307.	7.1	21
46	Generalized Entropy Theory of Glass Formation in Polymer Melts with Specific Interactions. Macromolecules, 2015, 48, 2333-2343.	4.8	29
47	Theory of competitive solvation of polymers by two solvents and entropy-enthalpy compensation in the solvation free energy upon dilution with the second solvent. Journal of Chemical Physics, 2015, 142, 214906.	3.0	13
48	Lattice cluster theory for dense, thin polymer films. Journal of Chemical Physics, 2015, 142, 134901.	3.0	2
49	Advances in the generalized entropy theory of glass-formation in polymer melts. Journal of Chemical Physics, 2014, 141, 234903.	3.0	35
50	Two glass transitions in miscible polymer blends?. Journal of Chemical Physics, 2014, 140, 244905.	3.0	25
51	Perturbative many-body expansion for electrostatic energy and field for system of polarizable charged spherical ions in a dielectric medium. Journal of Chemical Physics, 2014, 141, 034115.	3.0	15
52	Communication: Towards first principles theory of relaxation in supercooled liquids formulated in terms of cooperative motion. Journal of Chemical Physics, 2014, 141, 141102.	3.0	40
53	Concentration fluctuations in miscible polymer blends: Influence of temperature and chain rigidity. Journal of Chemical Physics, 2014, 140, 194901.	3.0	8
54	Lattice cluster theory for polymer melts with specific interactions. Journal of Chemical Physics, 2014, 141, 044909.	3.0	34

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55	Benchmarking all-atom simulations using hydrogen exchange. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15975-15980.	7.1	67
56	Loss of conformational entropy in protein folding calculated using realistic ensembles and its implications for NMR-based calculations. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15396-15401.	7.1	101
57	Influence of Cohesive Energy and Chain Stiffness on Polymer Glass Formation. Macromolecules, 2014, 47, 6990-6997.	4.8	61
58	Differences in Dynamics and Stability of the Wild Type Beta-Amyloid AÎ²1-40, and Î”E22-AÎ²1-39 (Japanese) Mutant Protofibril Structures, a Molecular Dynamics Study. Biophysical Journal, 2014, 106, 482a.	0.5	0
59	Simplified Protein Models: Predicting Folding Pathways and Structure Using Amino Acid Sequences. Physical Review Letters, 2013, 111, 028103.	7.8	30
60	A Novel Implicit Solvent Model for Simulating the Molecular Dynamics ofÂRNA. Biophysical Journal, 2013, 105, 1248-1257.	0.5	15
61	Molecular Origins of Cofilin-Linked Changes in Actin Filament Mechanics. Biophysical Journal, 2013, 104, 549a-550a.	0.5	0
62	Phase field method for nonequilibrium dynamics of reversible self-assembly systems. Journal of Chemical Physics, 2013, 139, 134904.	3.0	0
63	The Differences in Dynamics and Stability of the Wild Type Beta-Amyloid AÎ²1-40, and Î”E22-AÎ²1-39 (Japanese) Mutant, a Molecular Dynamics Study. Biophysical Journal, 2013, 104, 398a-399a.	0.5	0
64	Molecular Origins of Cofilin-Linked Changes in Actin Filament Mechanics. Journal of Molecular Biology, 2013, 425, 1225-1240.	4.2	44
65	Theoretical Studies of the Ground and Excited State Structures of Stilbene. Journal of Physical Chemistry A, 2013, 117, 9424-9434.	2.5	19
66	Thermodynamic scaling of dynamics in polymer melts: Predictions from the generalized entropy theory. Journal of Chemical Physics, 2013, 138, 234501.	3.0	21
67	Solvation of polymers as mutual association. I. General theory. Journal of Chemical Physics, 2013, 138, 164901.	3.0	7
68	Solvation of polymers as mutual association. II. Basic thermodynamic properties. Journal of Chemical Physics, 2013, 138, 164902.	3.0	12
69	Cooperativity in self-limiting equilibrium self-associating systems. Journal of Chemical Physics, 2012, 137, 204906.	3.0	3
70	Lattice cluster theory of associating polymers. I. Solutions of linear telechelic polymer chains. Journal of Chemical Physics, 2012, 136, 064902.	3.0	13
71	Influence of small rings on the thermodynamics of equilibrium self-assembly. Journal of Chemical Physics, 2012, 136, 244904.	3.0	9
72	Lattice cluster theory of associating telechelic polymers. III. Order parameter and average degree of self-assembly, transition temperature, and specific heat. Journal of Chemical Physics, 2012, 136, 194902.	3.0	5

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73	Lattice cluster theory of associating polymers. IV. Phase behavior of telechelic polymer solutions. Journal of Chemical Physics, 2012, 136, 194903.	3.0	4
74	De novo prediction of protein folding pathways and structure using the principle of sequential stabilization. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17442-17447.	7.1	44
75	Theoretical aids in screening candidates for atomic clocks: Illustration for Yb II. Europhysics Letters, 2012, 98, 23002.	2.0	2
76	The Relationship Between the Number of Residues in the Dynamics and Stability of the A-Beta Amyloid, a Molecular Dynamics Study. Biophysical Journal, 2012, 102, 631a.	0.5	0
77	Lattice cluster theory of associating polymers. II. Enthalpy and entropy of self-assembly and Flory-Huggins interaction parameter I‡ for solutions of telechelic molecules. Journal of Chemical Physics, 2012, 136, 064903.	3.0	11
78	Can the Miscibility of Telechelic Polymer Solutions Increase with Polymer Chain Length?. ACS Macro Letters, 2012, 1, 88-91.	4.8	5
79	The Folding Transition State of Protein L Is Extensive with Nonnative Interactions (and Not Small and) Tj ETQq1 1 0.784314 rgBT /Ove	4.2	28
80	Context and Force Field Dependence of the Loss of Protein Backbone Entropy upon Folding Using Realistic Denatured and Native State Ensembles. Journal of the American Chemical Society, 2012, 134, 15929-15936.	13.7	28
81	On Docking, Scoring and Assessing Protein-DNA Complexes in a Rigid-Body Framework. PLoS ONE, 2012, 7, e32647.	2.5	13
82	Modeling large regions in proteins: Applications to loops, termini, and folding. Protein Science, 2012, 21, 107-121.	7.6	17
83	Prediction of electronic structure of organic radicaloid anions using efficient, economical multireference gradient approach. Physical Chemistry Chemical Physics, 2011, 13, 7514.	2.8	18
84	The Descent into Glass Formation in Polymer Fluids. Accounts of Chemical Research, 2011, 44, 194-203.	15.6	34
85	Geometry Optimization of Radicaloid Systems Using Improved Virtual Orbital-Complete Active Space Configuration Interaction (IVO-CASCI) Analytical Gradient Method. Journal of Physical Chemistry A, 2011, 115, 3665-3678.	2.5	31
86	Comparison of Calculated and Measured Critical Flow Rates for Dragging Linear Polymer Chains through a Small Cylindrical Tube. Macromolecules, 2011, 44, 9863-9866.	4.8	20
87	Automated Real-Space Refinement of Protein Structures Using a Realistic Backbone Move Set. Biophysical Journal, 2011, 101, 899-909.	0.5	26
88	Modeling the Hydration Layer around Proteins: Applications to Small- and Wide-Angle X-Ray Scattering. Biophysical Journal, 2011, 101, 2061-2069.	0.5	66
89	Entropyâ^'Enthalpy Compensation in Chemical Reactions and Adsorption: An Exactly Solvable Model. Journal of Physical Chemistry B, 2011, 115, 1689-1692.	2.6	51
90	General approach to polymer chains confined by interacting boundaries. II. Flow through a cylindrical nano-tube. Journal of Chemical Physics, 2011, 135, 144902.	3.0	20

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91	Application of an efficient multireference approach to free-base porphin and metalloporphyrins: Ground, excited, and positive ion states. Journal of Chemical Physics, 2011, 135, 084118.	3.0	16
92	Protein structure prediction enhanced with evolutionary diversity: SPEED. Protein Science, 2010, 19, 520-534.	7.6	23
93	A Probabilistic and Continuous Model of Protein Conformational Space for Template-Free Modeling. Journal of Computational Biology, 2010, 17, 783-798.	1.6	16
94	Dynamics of electronic dephasing in the Fennaâ€"Matthewsâ€"Olson complex. New Journal of Physics, 2010, 12, 065042.	2.9	50
95	Molecular applications of analytical gradient approach for the improved virtual orbital-complete active space configuration interaction method. Journal of Chemical Physics, 2010, 132, 034105.	3.0	12
96	Electrostatic Solvation Energy for Two Oppositely Charged Ions in a Solvated Protein System: Salt Bridges Can Stabilize Proteins. Biophysical Journal, 2010, 98, 470-477.	0.5	24
97	Modeling the Hydration Layer around Proteins: HyPred. Biophysical Journal, 2010, 99, 1611-1619.	0.5	57
98	Plasticization and antiplasticization of polymer melts diluted by low molar mass species. Journal of Chemical Physics, 2010, 132, 084504.	3.0	76
99	Extended Structures in RNA Folding Intermediates Are Due to Nonnative Interactions Rather than Electrostatic Repulsion. Journal of Molecular Biology, 2010, 397, 1298-1306.	4.2	17
100	General approach to polymer chains confined by interacting boundaries. Journal of Chemical Physics, 2010, 133, 094901.	3.0	22
101	Langevin-Debye Model for Nonlinear Electrostatic Screening of Solvated Ions. Physical Review Letters, 2009, 102, 057603.	7.8	51
102	Crowding Induced Self-Assembly and Enthalpy-Entropy Compensation. Physical Review Letters, 2009, 103, 135701.	7.8	55
103	An exactly solvable model of hierarchical self-assembly. Journal of Chemical Physics, 2009, 130, 224906.	3.0	17
104	Mimicking the folding pathway to improve homology-free protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3734-3739.	7.1	59
105	Competition between self-assembly and surface adsorption. Journal of Chemical Physics, 2009, 130, 084903.	3.0	15
106	Extension of lattice cluster theory to strongly interacting, self-assembling polymeric systems. Journal of Chemical Physics, 2009, 130, 061103.	3.0	17
107	Equilibrium polymerization models of re-entrant self-assembly. Journal of Chemical Physics, 2009, 130, 164905.	3.0	20
108	Self-Assembly in a Polymer Matrix and Its Impact on Phase Separation. Journal of Physical Chemistry B, 2009, 113, 3920-3931.	2.6	18

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109	Ï‘-Constrained Simulations of Protein Folding Transition States: Implications for Calculating Ï•. Journal of Molecular Biology, 2009, 386, 920-928.	4.2	11
110	Application of the entropy theory of glass formation to poly(Î±-olefins). Journal of Chemical Physics, 2009, 131, 114905.	3.0	93
111	A Probabilistic Graphical Model for Ab Initio Folding. Lecture Notes in Computer Science, 2009, 5541, 59-73.	1.3	7
112	Quantifying the Structural Requirements of the Folding Transition State of Protein A and Other Systems. Journal of Molecular Biology, 2008, 381, 1362-1381.	4.2	31
113	Self-Assembly by Mutual Association: Basic Thermodynamic Properties. Journal of Physical Chemistry B, 2008, 112, 16193-16204.	2.6	34
114	Benchmarking Implicit Solvent Folding Simulations of the Amyloid Î²(10â^'35) Fragmentâ€. Journal of Physical Chemistry B, 2008, 112, 6175-6186.	2.6	30
115	Solvation effect on conformations of 1,2:dimethoxyethane: Charge-dependent nonlinear response in implicit solvent models. Journal of Chemical Physics, 2008, 128, 034501.	3.0	47
116	Potential energy curve for isomerization of N2H2 and C2H4 using the improved virtual orbital multireference MÃ¸llerâ€"Plesset perturbation theory. Journal of Chemical Physics, 2008, 128, 144304.	3.0	44
117	Lattice model of equilibrium polymerization. VII. Understanding the role of â€œcooperativityâ€•in self-assembly. Journal of Chemical Physics, 2008, 128, 224901.	3.0	65
118	Improved virtual orbital multireference MÃ¸llerâ€"Plesset study of the ground and excited electronic states of protonated acetylene, C2H3+. Journal of Chemical Physics, 2008, 129, 054308.	3.0	10
119	Multistep relaxation in equilibrium polymer solutions: A minimal model of relaxation in â€œcomplexâ€• fluids. Journal of Chemical Physics, 2008, 129, 094901.	3.0	35
120	Influence of nonlinear electrostatics on transfer energies between liquid phases: Charge burial is far less expensive than Born model. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 11146-11151.	7.1	54
121	Reappraisal ofciseffect in 1,2-dihaloethenes: An improved virtual orbital multireference approach. Journal of Chemical Physics, 2008, 129, 064101.	3.0	23
122	Lattice model of equilibrium polymerization. VI. Measures of fluid â€œcomplexityâ€•and search for generalized corresponding states. Journal of Chemical Physics, 2007, 127, 224901.	3.0	26
123	Functional Integrals and Polymer Statistics. Advances in Chemical Physics, 2007, , 1-128.	0.3	228
124	Photodissociation of Diatomic Molecules to Open Shell Atoms. Advances in Chemical Physics, 2007, , 1-113.	0.3	53
125	Lattice Cluster Theory of Multicomponent Polymer Systems: Chain Semiflexibility and Specific Interactions. Advances in Chemical Physics, 2007, , 335-390.	0.3	59
126	Collisional Effects on Electronic Relaxation Processes. Advances in Chemical Physics, 2007, , 207-269.	0.3	37

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127	Collision-Induced Intersystem Crossing. Advances in Chemical Physics, 2007, , 291-336.	0.3	38
128	Polypeptide Motions Are Dominated by Peptide Group Oscillations Resulting from Dihedral Angle Correlations between Nearest Neighborsâ€. Biochemistry, 2007, 46, 669-682.	2.5	31
129	The Algebra of Effective Hamiltonians and Operators: Exact Operators. Advances in Chemical Physics, 2007, , 465-541.	0.3	33
130	Actin polymerization under pressure: A theoretical study. Journal of Chemical Physics, 2007, 126, 024908.	3.0	5
131	Analysis and Evaluation of Ionization Potentials, Electron Affinities, and Excitation Energies by the Equations of Motion-Green's Function Method. Advances in Chemical Physics, 2007, , 1-69.	0.3	185
132	Geometry optimization using improved virtual orbitals: A complete active space numerical gradient approach. Journal of Chemical Physics, 2007, 126, 114103.	3.0	14
133	Reduced C_{Î²} statistical potentials can outperform allâ€atom potentials in decoy identification. Protein Science, 2007, 16, 2123-2139.	7.6	37
134	Small Proteins Fold Through Transition States With Native-like Topologies. Journal of Molecular Biology, 2006, 361, 755-770.	4.2	36
135	Minimalist Representations and the Importance of Nearest Neighbor Effects in Protein Folding Simulations. Journal of Molecular Biology, 2006, 363, 835-857.	4.2	40
136	Ab initio description of the ground and excited states of cyanogen isomers. Computational and Theoretical Chemistry, 2006, 768, 119-126.	1.5	13
137	Does equilibrium polymerization describe the dynamic heterogeneity of glass-forming liquids?. Journal of Chemical Physics, 2006, 125, 144907.	3.0	75
138	Minimal model of relaxation in an associating fluid: Viscoelastic and dielectric relaxations in equilibrium polymer solutions. Journal of Chemical Physics, 2006, 125, 184905.	3.0	16
139	Lattice model of equilibrium polymerization. V. Scattering properties and the width of the critical regime for phase separation. Journal of Chemical Physics, 2006, 124, 144906.	3.0	26
140	Entropy theory of polymer glass formation revisited. I. General formulation. Journal of Chemical Physics, 2006, 124, 064901.	3.0	85
141	A simple method for faster nonbonded force evaluations. Journal of Computational Chemistry, 2005, 26, 691-698.	3.3	16
142	Quadratic PadÃ© approximants and the intruder state problem of multireference perturbation methods. International Journal of Quantum Chemistry, 2005, 105, 18-33.	2.0	8
143	Compressible models of equilibrium polymerization. Journal of Chemical Physics, 2005, 123, 194906.	3.0	14
144	Electronic structure of the calcium monohydroxide radical. Journal of Chemical Physics, 2005, 122, 044317.	3.0	28

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145	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
146	Relativistic effective valence shell Hamiltonian method: Excitation and ionization energies of heavy metal atoms. Journal of Chemical Physics, 2005, 122, 204111.	3.0	20
147	Direct computation of characteristic temperatures and relaxation times for glass-forming polymer liquids. Journal of Chemical Physics, 2005, 123, 111102.	3.0	45
148	Statistical coil model of the unfolded state: Resolving the reconciliation problem. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13099-13104.	7.1	290
149	Generation of potential energy curves for the XÎ£g+1, BÎ”g+1, and Bâ€²Î£g+1 states of C2 using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 2005, 122, 154310.	3.0	11
150	The Glass Transition Temperature of Polymer Melts. Journal of Physical Chemistry B, 2005, 109, 21285-21292.	2.6	157
151	Fragility of Glass-Forming Polymer Liquids. Journal of Physical Chemistry B, 2005, 109, 21350-21356.	2.6	121
152	Helix, Sheet, and Polyproline II Frequencies and Strong Nearest Neighbor Effects in a Restricted Coil Library. Biochemistry, 2005, 44, 9691-9702.	2.5	165
153	Flory-Huggins Model of Equilibrium Polymerization and Phase Separation in the Stockmayer Fluid. Physical Review Letters, 2004, 92, 045502.	7.8	64
154	Analytic density-functional self-consistent-field theory of diblock copolymers near patterned surfaces. Journal of Chemical Physics, 2004, 120, 7174-7182.	3.0	10
155	Mixtures of lattice polymers with structured monomers. Journal of Chemical Physics, 2004, 120, 6288-6298.	3.0	4
156	Influence of Frequency Shifts on Electron Transfer Processes. Journal of Physical Chemistry B, 2003, 107, 10341-10343.	2.6	27
157	Large-Scale Context in Protein Folding:Â Villin Headpieceâ€. Biochemistry, 2003, 42, 664-671.	2.5	56
158	Computer Simulation of Met-Enkephalin Using Explicit Atom and United Atom Potentials:â€‰ Similarities, Differences, and Suggestions for Improvement. Journal of Physical Chemistry B, 2003, 107, 1685-1691.	2.6	27
159	Investigations into Sequence and Conformational Dependence of Backbone Entropy, Inter-basin Dynamics and the Flory Isolated-pair Hypothesis for Peptides. Journal of Molecular Biology, 2003, 331, 693-711.	4.2	118
160	Folding and misfolding of the papillomavirus E6 interacting peptide E6ap. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 7087-7092.	7.1	11
161	A critical analysis of the ground and excited electronic states of transition metal nitrides using the relativistic effective Hamiltonian method. Journal of Chemical Physics, 2003, 119, 5995-6002.	3.0	11
162	Lattice model of equilibrium polymerization. IV. Influence of activation, chemical initiation, chain scission and fusion, and chain stiffness on polymerization and phase separation. Journal of Chemical Physics, 2003, 119, 12645-12666.	3.0	87

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163	Influence of monomer molecular structure on the glass transition in polymers I. Lattice cluster theory for the configurational entropy. Journal of Chemical Physics, 2003, 119, 5730-5739.	3.0	41
164	The effective valence shell Hamiltonian for spin-orbit coupling. Journal of Chemical Physics, 2003, 118, 8281-8289.	3.0	6
165	Long time dynamics of Met-enkephalin: Tests of mode-coupling theory and implicit solvent models. Journal of Chemical Physics, 2003, 118, 5143-5156.	3.0	12
166	The polymerization of actin: Thermodynamics near the polymerization line. Journal of Chemical Physics, 2003, 119, 4070-4084.	3.0	40
167	Hydration structure of met-enkephalin: A molecular dynamics study. Journal of Chemical Physics, 2003, 118, 1989-1995.	3.0	10
168	Lattice polymers with structured monomers: A Monte Carlo study of thermodynamic properties of melts and solutions. Journal of Chemical Physics, 2002, 116, 10959-10966.	3.0	10
169	Analytical solution for steady-state populations in the self-assembly of microtubules from nucleating sites. Physical Review E, 2002, 66, 061916.	2.1	14
170	Liquid-state theory derivation of surface accessible solvation potential models for proteins. Journal of Chemical Physics, 2002, 116, 10475-10477.	3.0	4
171	A comparison of self-assembly in lattice and off-lattice model amphiphile solutions. Journal of Chemical Physics, 2002, 116, 4765.	3.0	11
172	The Excited and Ion States of Allene. ACS Symposium Series, 2002, , 154-175.	0.5	5
173	Beyond Flory-Huggins Theory: New Classes of Blend Miscibility Associated with Monomer Structural Asymmetry. Physical Review Letters, 2002, 88, 095503.	7.8	43
174	New patterns of polymer blend miscibility associated with monomer shape and size asymmetry. Journal of Chemical Physics, 2002, 116, 9983-9996.	3.0	37
175	Small angle neutron scattering studies of a polybutadiene/polystyrene blend with small additions of ortho-dichloro-benzene for varying temperatures and pressures. II. Phase boundaries and Floryâ€"Huggins parameter. Journal of Chemical Physics, 2002, 116, 2241-2250.	3.0	9
176	Vector properties of S(3P) and S(1D) in the photodissociation of SH: Quantum interference and overlapping resonance. Journal of Chemical Physics, 2002, 116, 10656-10663.	3.0	11
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